Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 03:51 AM UTC

PDB ID	:	9DKN / pdb_00009dkn
EMDB ID	:	EMD-46963
Title	:	Apo aplysia Slo1 R202Q
Authors	:	Gustavo, G.F.; Shen, R.; Latorre, R.; Perozo, E.
Deposited on	:	2024-09-09
Resolution	:	3.50 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

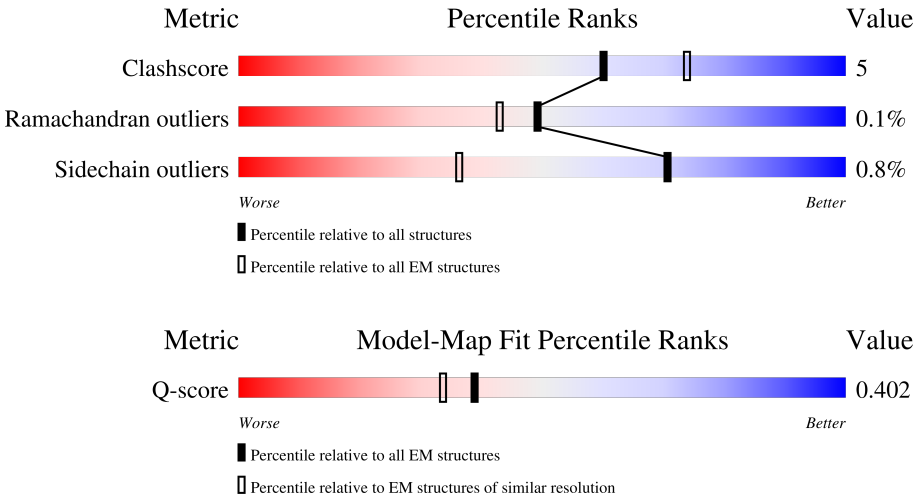
EMDB validation analysis	:	0.0.1.dev132
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13950 (3.00 - 4.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1065	7% 78% 6% 16%
1	B	1065	7% 77% 7% • 16%
1	C	1065	7% 78% 7% 16%
1	D	1065	7% 78% 6% 16%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 28376 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called BK channel.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	899	Total	C	N	O	S	0	0
			7094	4603	1158	1290	43		
1	B	899	Total	C	N	O	S	0	0
			7094	4603	1158	1290	43		
1	C	899	Total	C	N	O	S	0	0
			7094	4603	1158	1290	43		
1	D	899	Total	C	N	O	S	0	0
			7094	4603	1158	1290	43		

There are 8 discrepancies between the modelled and reference sequences:

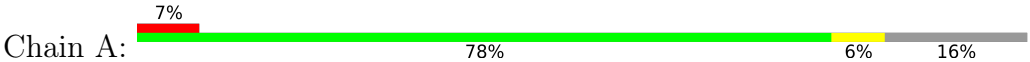
Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ALA	THR	engineered mutation	UNP Q5QJC5
A	202	GLN	ARG	engineered mutation	UNP Q5QJC5
B	2	ALA	THR	engineered mutation	UNP Q5QJC5
B	202	GLN	ARG	engineered mutation	UNP Q5QJC5
C	2	ALA	THR	engineered mutation	UNP Q5QJC5
C	202	GLN	ARG	engineered mutation	UNP Q5QJC5
D	2	ALA	THR	engineered mutation	UNP Q5QJC5
D	202	GLN	ARG	engineered mutation	UNP Q5QJC5

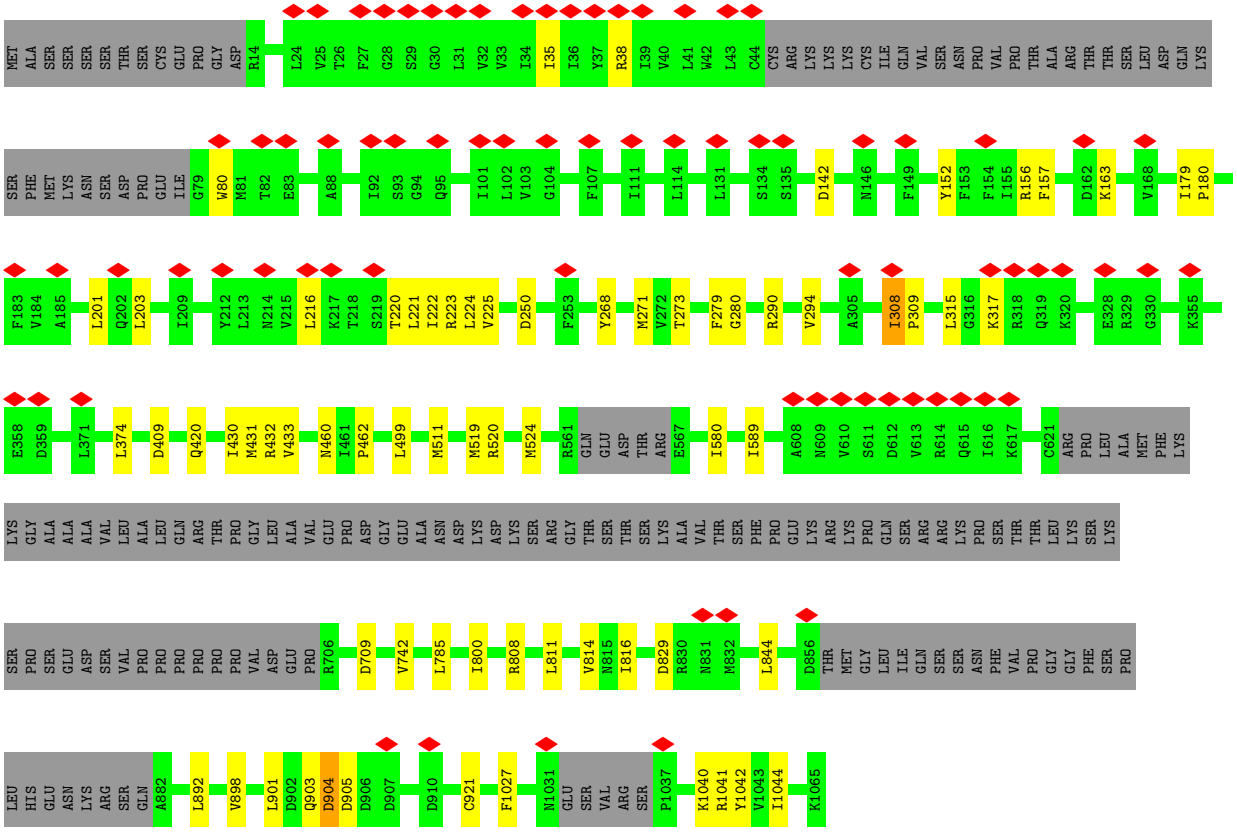
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: BK channel

Chain A:

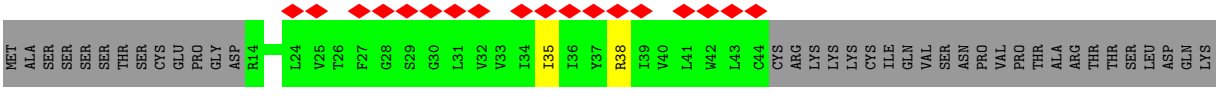


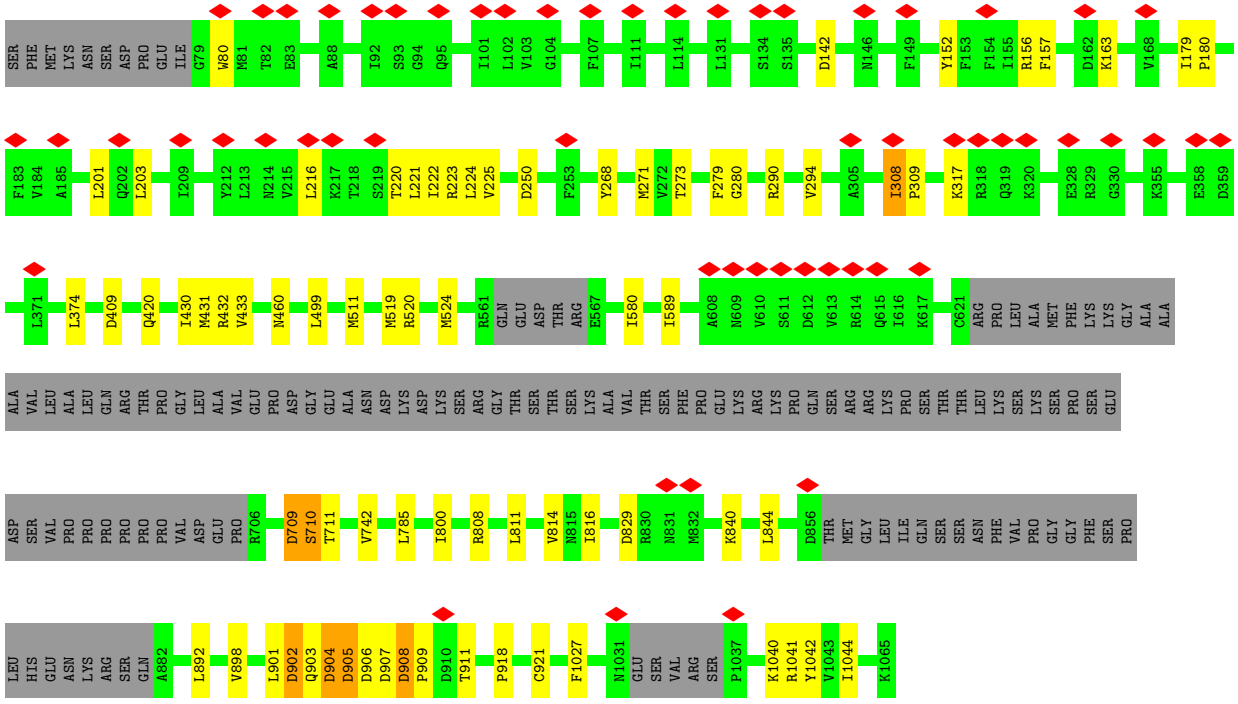


• Molecule 1: BK channel

Chain B:



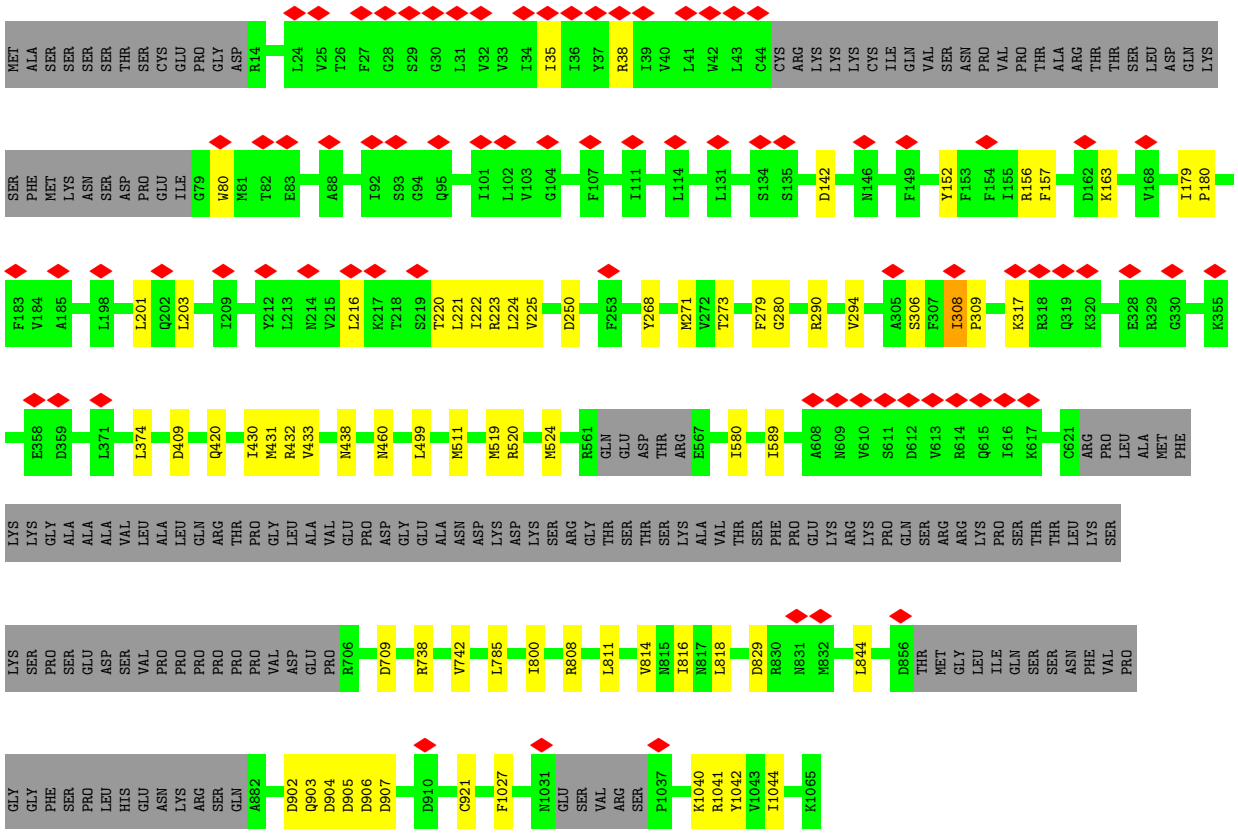




• Molecule 1: BK channel

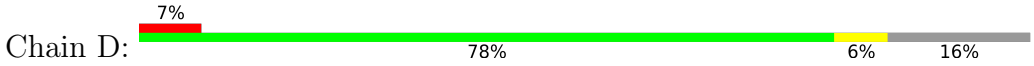
Chain C:

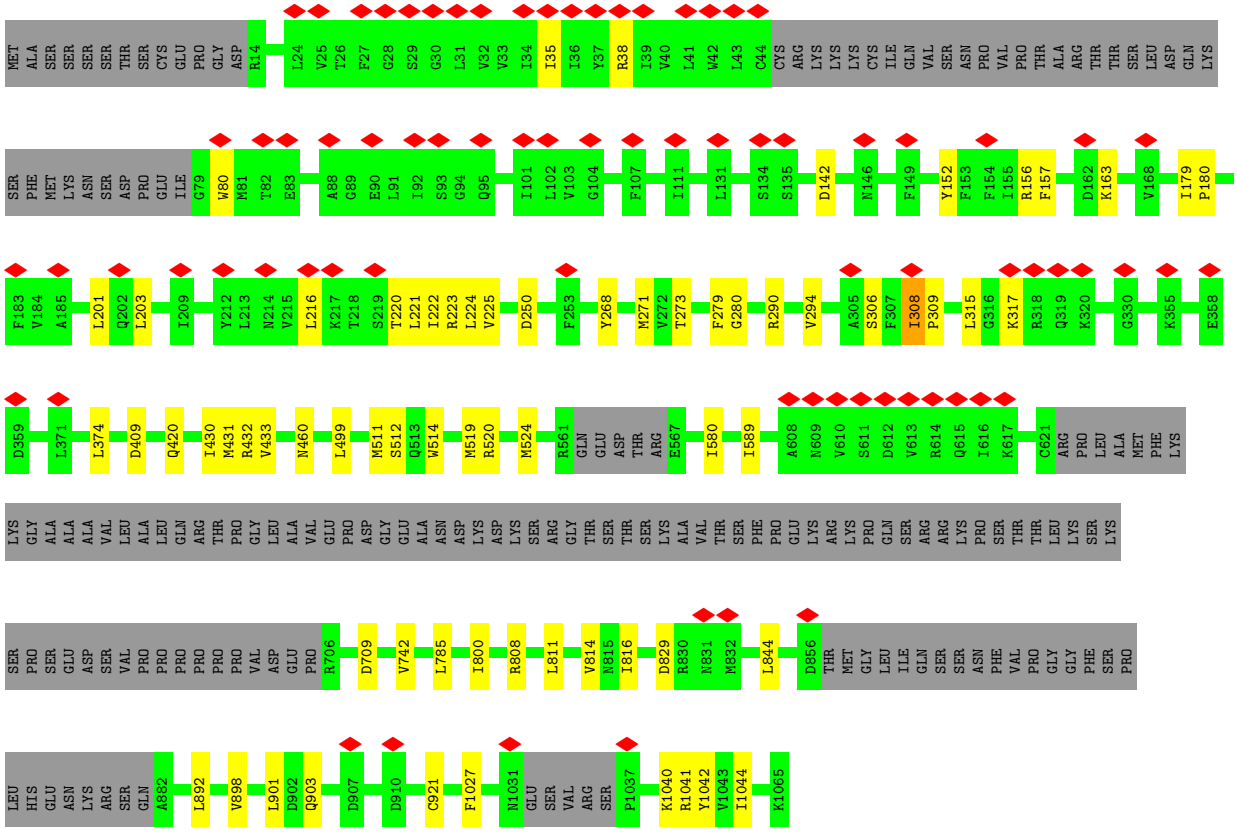




• Molecule 1: BK channel

Chain D:


7%
78%
6%
16%


MET ALA SER SER SER THR SER CYS GLU PRO GLY ASP R14 L24 V25 T26 F27 G28 S29 G30 L31 V32 V33 I34 I35 I36 Y37 R38 I39 V40 L41 W42 L43 C44 CYS ARG LYS LYS LYS CYS ILE GLN VAL SER ASN PRO VAL PRO THR ALA ARG THR THR SER LEU ASP GLN LYS
SER PHE MET LYS ASN SER ASP PRO GLU ILE G79 W80 M81 T82 E83 A88 G89 E90 L91 I92 S93 G94 Q95 I101 L102 V103 G104 F107 I111 L131 S134 S135 D142 N146 F149 Y152 F153 F154 I155 R156 F157 D162 K163 V168 I179 P180
F183 V184 A185 L201 Q202 L203 I209 Y212 L213 N214 V215 L216 K217 T218 S219 T220 L221 I222 R223 L224 V225 D250 F253 Y268 M271 V272 T273 F279 G280 R290 V294 A305 S306 F307 I308 P309 L315 G316 K317 R318 Q319 K320 G330 K355 E358
D359 L371 L374 D409 Q420 I430 M431 R432 V433 N460 L499 M511 S512 Q513 W514 M519 R520 M524 R561 GLN GLU ASP THR ARG E567 I580 I589 A608 N609 V610 S611 D612 V613 R614 Q615 I616 K617 C621 ARG PRO LEU ALA MET PHE LYS
LYS GLY ALA ALA ALA VAL LEU ALA LEU GLN ARG THR PRO GLY LEU ALA VAL GLU PRO ASP GLY GLU ALA ASN ASP LYS ASP LYS SER ARG GLY THR SER THR SER LYS ALA VAL THR SER PHE PRO GLU LYS ARG LYS PRO GLN SER ARG ARG LYS PRO SER THR THR LEU LYS SER LYS
SER PRO SER GLU ASP SER VAL PRO PRO PRO PRO PRO VAL ASP GLU PRO R706 D709 V742 L785 I800 R808 L811 V814 N815 I816 D829 R830 N831 M832 L844 D856 THR MET GLY LEU ILE GLN SER SER ASN PHE VAL PRO GLY GLY PHE SER PRO
LEU HIS GLU ASN LYS ARG SER GLN A882 L892 V898 L901 D902 Q903 D907 D910 C921 F1027 N1031 GLU SER VAL ARG SER P1037 K1040 R1041 Y1042 Y1043 I1044 K1065

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	50420	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	65	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.091	Depositor
Minimum map value	-0.461	Depositor
Average map value	0.012	Depositor
Map value standard deviation	0.057	Depositor
Recommended contour level	0.259	Depositor
Map size (Å)	274.432, 274.432, 274.432	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.072, 1.072, 1.072	Depositor

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.72	0/7265	1.22	7/9876 (0.1%)
1	B	0.72	0/7265	1.21	7/9876 (0.1%)
1	C	0.72	0/7265	1.21	8/9876 (0.1%)
1	D	0.72	0/7265	1.22	7/9876 (0.1%)
All	All	0.72	0/29060	1.22	29/39504 (0.1%)

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	829	ASP	N-CA-C	-6.62	101.79	110.53
1	A	829	ASP	N-CA-C	-6.60	101.82	110.53
1	D	829	ASP	N-CA-C	-6.58	101.84	110.53
1	B	829	ASP	N-CA-C	-6.58	101.84	110.53
1	A	308	ILE	O-C-N	6.26	124.43	120.42
1	C	308	ILE	O-C-N	6.26	124.43	120.42
1	D	308	ILE	O-C-N	6.15	124.36	120.42
1	B	308	ILE	O-C-N	6.10	124.32	120.42
1	C	409	ASP	CA-CB-CG	5.67	118.27	112.60
1	A	409	ASP	CA-CB-CG	5.64	118.24	112.60
1	D	142	ASP	CA-CB-CG	5.63	118.23	112.60
1	A	142	ASP	CA-CB-CG	5.63	118.23	112.60
1	B	142	ASP	CA-CB-CG	5.58	118.18	112.60
1	B	409	ASP	CA-CB-CG	5.58	118.18	112.60
1	D	409	ASP	CA-CB-CG	5.58	118.18	112.60
1	C	142	ASP	CA-CB-CG	5.56	118.16	112.60
1	C	906	ASP	N-CA-C	-5.54	106.02	112.89
1	A	250	ASP	CA-CB-CG	5.41	118.00	112.60
1	C	250	ASP	CA-CB-CG	5.40	118.00	112.60
1	B	250	ASP	CA-CB-CG	5.40	118.00	112.60
1	D	250	ASP	CA-CB-CG	5.37	117.97	112.60
1	C	80	TRP	CA-C-N	5.20	127.50	120.38
1	C	80	TRP	C-N-CA	5.20	127.50	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	80	TRP	CA-C-N	5.18	127.48	120.38
1	D	80	TRP	C-N-CA	5.18	127.48	120.38
1	A	80	TRP	CA-C-N	5.16	127.45	120.38
1	A	80	TRP	C-N-CA	5.16	127.45	120.38
1	B	80	TRP	CA-C-N	5.13	127.42	120.38
1	B	80	TRP	C-N-CA	5.13	127.42	120.38

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7094	0	6980	88	0
1	B	7094	0	6980	88	0
1	C	7094	0	6980	82	0
1	D	7094	0	6980	85	0
All	All	28376	0	27920	255	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (255) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:524:MET:CE	1:B:589:ILE:HG22	1.81	1.11
1:D:524:MET:CE	1:D:589:ILE:HG22	1.81	1.10
1:C:524:MET:CE	1:C:589:ILE:HG22	1.81	1.09
1:A:524:MET:CE	1:A:589:ILE:HG22	1.81	1.08
1:B:524:MET:HE2	1:B:589:ILE:HG22	1.42	0.99
1:A:524:MET:HE2	1:A:589:ILE:HG22	1.42	0.99
1:C:524:MET:HE2	1:C:589:ILE:HG22	1.42	0.99
1:C:273:THR:HG22	1:D:279:PHE:CE1	1.98	0.98
1:D:524:MET:HE2	1:D:589:ILE:HG22	1.42	0.98
1:B:273:THR:HG22	1:C:279:PHE:CE1	1.99	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:THR:HG22	1:B:279:PHE:CE1	1.98	0.97
1:D:216:LEU:HD11	1:D:225:VAL:HG21	1.49	0.95
1:C:216:LEU:HD11	1:C:225:VAL:HG21	1.49	0.94
1:B:216:LEU:HD11	1:B:225:VAL:HG21	1.49	0.94
1:A:216:LEU:HD11	1:A:225:VAL:HG21	1.49	0.94
1:B:216:LEU:HD22	1:B:221:LEU:HD23	1.53	0.90
1:A:216:LEU:HD22	1:A:221:LEU:HD23	1.53	0.90
1:C:216:LEU:HD22	1:C:221:LEU:HD23	1.53	0.90
1:B:216:LEU:CD2	1:B:221:LEU:HD23	2.03	0.88
1:D:216:LEU:HD22	1:D:221:LEU:HD23	1.53	0.88
1:A:216:LEU:CD1	1:A:225:VAL:HG21	2.04	0.88
1:A:279:PHE:CE1	1:D:273:THR:HG22	2.09	0.88
1:D:216:LEU:CD1	1:D:225:VAL:HG21	2.04	0.87
1:B:216:LEU:CD1	1:B:225:VAL:HG21	2.04	0.87
1:C:216:LEU:CD1	1:C:225:VAL:HG21	2.04	0.87
1:D:216:LEU:CD2	1:D:221:LEU:HD23	2.03	0.87
1:A:216:LEU:CD2	1:A:221:LEU:HD23	2.03	0.87
1:C:216:LEU:CD2	1:C:221:LEU:HD23	2.03	0.86
1:C:273:THR:CG2	1:D:279:PHE:CE1	2.59	0.86
1:A:271:MET:HG2	1:D:294:VAL:HG13	1.59	0.85
1:B:273:THR:CG2	1:C:279:PHE:CE1	2.61	0.84
1:C:294:VAL:HG13	1:D:271:MET:HG2	1.59	0.84
1:A:273:THR:CG2	1:B:279:PHE:CE1	2.61	0.82
1:A:374:LEU:HD13	1:D:317:LYS:NZ	1.96	0.81
1:B:294:VAL:HG13	1:C:271:MET:HG2	1.63	0.79
1:A:808:ARG:HH12	1:D:460:ASN:HD21	1.29	0.79
1:B:273:THR:CG2	1:C:279:PHE:CZ	2.66	0.79
1:A:273:THR:CG2	1:B:279:PHE:CZ	2.67	0.78
1:C:273:THR:CG2	1:D:279:PHE:CZ	2.65	0.78
1:A:273:THR:HG22	1:B:279:PHE:HE1	1.47	0.78
1:B:273:THR:HG22	1:C:279:PHE:HE1	1.49	0.77
1:D:524:MET:HE2	1:D:589:ILE:CG2	2.14	0.77
1:A:273:THR:HG22	1:B:279:PHE:CZ	2.20	0.77
1:A:294:VAL:HG13	1:B:271:MET:HG2	1.66	0.77
1:B:524:MET:HE2	1:B:589:ILE:CG2	2.14	0.77
1:C:524:MET:HE2	1:C:589:ILE:CG2	2.14	0.76
1:A:524:MET:HE2	1:A:589:ILE:CG2	2.14	0.76
1:A:462:PRO:HG2	1:B:903:GLN:HG2	1.68	0.75
1:A:279:PHE:CE1	1:D:273:THR:CG2	2.69	0.75
1:C:273:THR:HG22	1:D:279:PHE:CZ	2.21	0.75
1:B:273:THR:HG22	1:C:279:PHE:CZ	2.21	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:524:MET:CE	1:D:589:ILE:CG2	2.65	0.74
1:C:273:THR:HG22	1:D:279:PHE:HE1	1.48	0.74
1:B:524:MET:CE	1:B:589:ILE:CG2	2.65	0.74
1:A:808:ARG:HH12	1:D:460:ASN:ND2	1.86	0.73
1:A:374:LEU:HD13	1:D:317:LYS:HZ1	1.53	0.73
1:A:808:ARG:NH1	1:D:460:ASN:HD21	1.86	0.73
1:A:524:MET:CE	1:A:589:ILE:CG2	2.65	0.72
1:C:524:MET:CE	1:C:589:ILE:CG2	2.65	0.72
1:A:317:LYS:HZ1	1:B:374:LEU:HD13	1.57	0.70
1:B:317:LYS:NZ	1:C:374:LEU:HD13	2.07	0.70
1:A:279:PHE:CZ	1:D:273:THR:CG2	2.75	0.69
1:C:317:LYS:NZ	1:D:374:LEU:HD13	2.07	0.69
1:C:273:THR:HG21	1:D:279:PHE:CZ	2.28	0.69
1:A:317:LYS:NZ	1:B:374:LEU:HD13	2.07	0.68
1:A:279:PHE:HE1	1:D:273:THR:HG22	1.56	0.68
1:A:273:THR:CG2	1:B:279:PHE:HE1	2.04	0.68
1:D:524:MET:HE3	1:D:589:ILE:HG22	1.74	0.68
1:C:273:THR:CG2	1:D:279:PHE:HE1	2.02	0.68
1:A:460:ASN:HD21	1:B:808:ARG:NH1	1.93	0.67
1:A:524:MET:HE3	1:A:589:ILE:HG22	1.74	0.67
1:B:273:THR:HG21	1:C:279:PHE:CZ	2.30	0.67
1:A:460:ASN:HD21	1:B:808:ARG:HH12	1.42	0.67
1:A:279:PHE:CZ	1:D:273:THR:HG22	2.31	0.66
1:B:460:ASN:HD21	1:C:808:ARG:HH12	1.44	0.66
1:C:317:LYS:HZ1	1:D:374:LEU:HD13	1.61	0.66
1:C:460:ASN:HD21	1:D:808:ARG:HH12	1.44	0.66
1:C:811:LEU:O	1:C:816:ILE:HG12	1.96	0.66
1:A:811:LEU:O	1:A:816:ILE:HG12	1.97	0.65
1:A:273:THR:HG21	1:B:279:PHE:CZ	2.31	0.65
1:D:811:LEU:O	1:D:816:ILE:HG12	1.97	0.65
1:B:892:LEU:HD21	1:B:901:LEU:HD11	1.77	0.65
1:C:273:THR:HG21	1:D:279:PHE:HZ	1.62	0.65
1:D:512:SER:HG	1:D:514:TRP:CD1	2.15	0.65
1:A:279:PHE:HE1	1:D:273:THR:CG2	2.10	0.64
1:C:524:MET:HE3	1:C:589:ILE:HG22	1.73	0.64
1:B:273:THR:CG2	1:C:279:PHE:HE1	2.04	0.64
1:B:811:LEU:O	1:B:816:ILE:HG12	1.97	0.64
1:B:317:LYS:HZ1	1:C:374:LEU:HD13	1.63	0.63
1:B:524:MET:HE3	1:B:589:ILE:HG22	1.74	0.63
1:C:438:ASN:HA	1:D:903:GLN:HE22	1.63	0.63
1:B:273:THR:HG21	1:C:279:PHE:HZ	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:898:VAL:HA	1:D:901:LEU:HD13	1.82	0.62
1:A:460:ASN:ND2	1:B:808:ARG:HH12	1.97	0.62
1:A:273:THR:HG21	1:B:279:PHE:HZ	1.66	0.61
1:B:709:ASP:O	1:B:710:SER:C	2.43	0.61
1:B:460:ASN:HD21	1:C:808:ARG:NH1	1.99	0.61
1:A:898:VAL:HA	1:A:901:LEU:HD13	1.83	0.61
1:C:460:ASN:HD21	1:D:808:ARG:NH1	1.99	0.61
1:A:808:ARG:NH1	1:D:460:ASN:ND2	2.48	0.60
1:C:273:THR:CG2	1:D:279:PHE:HZ	2.14	0.60
1:A:279:PHE:CZ	1:D:273:THR:HG21	2.37	0.60
1:A:268:TYR:CE2	1:D:290:ARG:NH2	2.71	0.59
1:B:460:ASN:ND2	1:C:808:ARG:HH12	2.00	0.58
1:B:785:LEU:HD13	1:B:800:ILE:HG21	1.84	0.58
1:A:892:LEU:HD21	1:A:901:LEU:HD11	1.85	0.58
1:A:785:LEU:HD13	1:A:800:ILE:HG21	1.85	0.58
1:D:785:LEU:HD13	1:D:800:ILE:HG21	1.84	0.58
1:A:273:THR:CG2	1:B:279:PHE:HZ	2.15	0.58
1:C:460:ASN:ND2	1:D:808:ARG:HH12	2.00	0.58
1:C:785:LEU:HD13	1:C:800:ILE:HG21	1.85	0.58
1:B:273:THR:CG2	1:C:279:PHE:HZ	2.15	0.57
1:C:785:LEU:HD13	1:C:800:ILE:CG2	2.35	0.56
1:A:785:LEU:HD13	1:A:800:ILE:CG2	2.35	0.56
1:B:785:LEU:HD13	1:B:800:ILE:CG2	2.35	0.56
1:D:785:LEU:HD13	1:D:800:ILE:CG2	2.35	0.56
1:A:279:PHE:HZ	1:D:273:THR:HG21	1.69	0.56
1:B:902:ASP:HB3	1:B:918:PRO:HG3	1.87	0.56
1:B:903:GLN:O	1:B:904:ASP:C	2.48	0.56
1:C:290:ARG:NH2	1:D:268:TYR:CE2	2.75	0.55
1:A:374:LEU:HD13	1:D:317:LYS:HZ3	1.72	0.55
1:A:460:ASN:ND2	1:B:808:ARG:NH1	2.54	0.55
1:D:742:VAL:HG21	1:D:816:ILE:HD13	1.89	0.55
1:B:742:VAL:HG21	1:B:816:ILE:HD13	1.89	0.55
1:C:280:GLY:HA3	1:D:279:PHE:O	2.06	0.54
1:A:742:VAL:HG21	1:A:816:ILE:HD13	1.89	0.54
1:C:742:VAL:HG21	1:C:816:ILE:HD13	1.89	0.54
1:A:216:LEU:HD22	1:A:221:LEU:HB3	1.90	0.53
1:C:519:MET:O	1:C:520:ARG:C	2.50	0.53
1:A:844:LEU:HD21	1:D:430:ILE:HG21	1.89	0.53
1:B:216:LEU:HD22	1:B:221:LEU:HB3	1.90	0.53
1:B:280:GLY:HA3	1:C:279:PHE:O	2.08	0.53
1:D:519:MET:O	1:D:520:ARG:C	2.51	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:290:ARG:NH2	1:C:268:TYR:CE2	2.77	0.52
1:D:216:LEU:HD22	1:D:221:LEU:HB3	1.90	0.52
1:A:279:PHE:O	1:D:280:GLY:HA3	2.10	0.52
1:A:430:ILE:HG21	1:B:844:LEU:HD21	1.91	0.52
1:B:898:VAL:HA	1:B:901:LEU:HD13	1.91	0.52
1:A:223:ARG:O	1:A:224:LEU:C	2.52	0.51
1:C:216:LEU:HD22	1:C:221:LEU:HB3	1.91	0.51
1:D:223:ARG:O	1:D:224:LEU:C	2.52	0.51
1:A:279:PHE:HZ	1:D:273:THR:CG2	2.23	0.51
1:C:223:ARG:O	1:C:224:LEU:C	2.52	0.51
1:C:308:ILE:N	1:C:309:PRO:HD2	2.27	0.50
1:D:308:ILE:N	1:D:309:PRO:HD2	2.26	0.50
1:A:308:ILE:N	1:A:309:PRO:HD2	2.26	0.50
1:B:709:ASP:O	1:B:711:THR:N	2.45	0.50
1:D:152:TYR:CD2	1:D:156:ARG:NH2	2.80	0.50
1:A:280:GLY:HA3	1:B:279:PHE:O	2.11	0.50
1:C:152:TYR:CD2	1:C:156:ARG:NH2	2.80	0.50
1:A:216:LEU:HD23	1:A:221:LEU:HD23	1.93	0.49
1:B:308:ILE:N	1:B:309:PRO:HD2	2.26	0.49
1:B:524:MET:HE3	1:B:589:ILE:CG2	2.40	0.49
1:B:216:LEU:HD23	1:B:221:LEU:HD23	1.93	0.49
1:C:524:MET:HE3	1:C:589:ILE:CG2	2.40	0.49
1:A:152:TYR:CD2	1:A:156:ARG:NH2	2.80	0.49
1:A:519:MET:O	1:A:520:ARG:C	2.50	0.49
1:B:152:TYR:CD2	1:B:156:ARG:NH2	2.80	0.49
1:B:223:ARG:O	1:B:224:LEU:C	2.52	0.49
1:D:216:LEU:HD23	1:D:221:LEU:HD23	1.92	0.48
1:B:460:ASN:ND2	1:C:808:ARG:NH1	2.60	0.48
1:B:519:MET:O	1:B:520:ARG:C	2.51	0.48
1:A:524:MET:HE3	1:A:589:ILE:CG2	2.39	0.48
1:D:524:MET:HE3	1:D:589:ILE:CG2	2.40	0.47
1:C:216:LEU:HD23	1:C:221:LEU:HD23	1.93	0.47
1:A:290:ARG:NH2	1:B:268:TYR:CE2	2.82	0.47
1:B:216:LEU:HD11	1:B:225:VAL:CG2	2.35	0.47
1:A:374:LEU:CD1	1:D:317:LYS:HZ3	2.28	0.47
1:B:430:ILE:HG21	1:C:844:LEU:HD21	1.97	0.47
1:D:216:LEU:HD22	1:D:221:LEU:CD2	2.36	0.47
1:D:892:LEU:HD21	1:D:901:LEU:HD11	1.97	0.47
1:B:216:LEU:HD22	1:B:221:LEU:CD2	2.36	0.47
1:C:216:LEU:CD1	1:C:225:VAL:CG2	2.87	0.47
1:B:222:ILE:O	1:B:223:ARG:C	2.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:903:GLN:O	1:C:904:ASP:C	2.57	0.46
1:D:216:LEU:HD11	1:D:225:VAL:CG2	2.35	0.46
1:D:222:ILE:O	1:D:223:ARG:C	2.58	0.46
1:D:430:ILE:O	1:D:431:MET:C	2.58	0.46
1:C:222:ILE:O	1:C:223:ARG:C	2.58	0.46
1:C:460:ASN:ND2	1:D:808:ARG:NH1	2.60	0.46
1:D:432:ARG:O	1:D:433:VAL:C	2.58	0.46
1:C:430:ILE:O	1:C:431:MET:C	2.58	0.46
1:A:814:VAL:HG23	1:A:816:ILE:CD1	2.46	0.46
1:A:844:LEU:HD21	1:D:430:ILE:CG2	2.46	0.46
1:C:430:ILE:HG21	1:D:844:LEU:HD21	1.98	0.46
1:D:1027:PHE:CE1	1:D:1041:ARG:NH2	2.84	0.45
1:B:499:LEU:HD11	1:B:589:ILE:CD1	2.47	0.45
1:C:499:LEU:HD11	1:C:589:ILE:CD1	2.47	0.45
1:A:499:LEU:HD11	1:A:589:ILE:CD1	2.47	0.45
1:B:1027:PHE:CE1	1:B:1041:ARG:NH2	2.84	0.45
1:A:430:ILE:O	1:A:431:MET:C	2.58	0.45
1:A:921:CYS:SG	1:A:1040:LYS:HE2	2.57	0.45
1:A:1027:PHE:CE1	1:A:1041:ARG:NH2	2.84	0.45
1:C:921:CYS:SG	1:C:1040:LYS:HE2	2.57	0.45
1:C:1027:PHE:CE1	1:C:1041:ARG:NH2	2.84	0.45
1:D:216:LEU:CD1	1:D:225:VAL:CG2	2.88	0.45
1:C:1042:TYR:CE2	1:C:1044:ILE:HD11	2.52	0.45
1:D:499:LEU:HD11	1:D:589:ILE:CD1	2.47	0.45
1:D:921:CYS:SG	1:D:1040:LYS:HE2	2.57	0.45
1:C:905:ASP:CG	1:C:907:ASP:H	2.25	0.45
1:B:814:VAL:HG23	1:B:816:ILE:CD1	2.46	0.45
1:B:921:CYS:SG	1:B:1040:LYS:HE2	2.57	0.45
1:C:814:VAL:HG23	1:C:816:ILE:CD1	2.46	0.45
1:D:814:VAL:HG23	1:D:816:ILE:CD1	2.46	0.45
1:B:511:MET:CE	1:B:519:MET:HE3	2.47	0.45
1:D:1042:TYR:CE2	1:D:1044:ILE:HD11	2.52	0.45
1:B:907:ASP:O	1:B:908:ASP:C	2.60	0.44
1:A:216:LEU:HD11	1:A:225:VAL:CG2	2.35	0.44
1:A:222:ILE:O	1:A:223:ARG:C	2.58	0.44
1:A:511:MET:CE	1:A:519:MET:HE3	2.47	0.44
1:C:511:MET:CE	1:C:519:MET:HE3	2.47	0.44
1:D:511:MET:CE	1:D:519:MET:HE3	2.47	0.44
1:B:1042:TYR:CE2	1:B:1044:ILE:HD11	2.52	0.44
1:B:432:ARG:O	1:B:433:VAL:C	2.58	0.44
1:A:1042:TYR:CE2	1:A:1044:ILE:HD11	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:430:ILE:O	1:B:431:MET:C	2.58	0.44
1:B:908:ASP:N	1:B:909:PRO:HD3	2.33	0.44
1:A:432:ARG:O	1:A:433:VAL:C	2.58	0.44
1:A:216:LEU:HD22	1:A:221:LEU:CD2	2.36	0.43
1:A:903:GLN:O	1:A:904:ASP:C	2.61	0.43
1:C:216:LEU:HD22	1:C:221:LEU:CD2	2.36	0.43
1:B:179:ILE:HB	1:B:180:PRO:HD3	2.01	0.42
1:B:216:LEU:CD1	1:B:225:VAL:CG2	2.87	0.42
1:C:432:ARG:O	1:C:433:VAL:C	2.58	0.42
1:C:179:ILE:HB	1:C:180:PRO:HD3	2.01	0.42
1:C:317:LYS:HZ3	1:D:374:LEU:HD13	1.84	0.42
1:D:179:ILE:HB	1:D:180:PRO:HD3	2.01	0.42
1:A:179:ILE:HB	1:A:180:PRO:HD3	2.02	0.42
1:A:431:MET:HE3	1:B:840:LYS:HG2	2.01	0.42
1:B:220:THR:O	1:B:224:LEU:HD13	2.20	0.42
1:C:156:ARG:O	1:C:157:PHE:C	2.63	0.42
1:B:156:ARG:O	1:B:157:PHE:C	2.63	0.42
1:D:220:THR:O	1:D:224:LEU:HD13	2.20	0.42
1:A:157:PHE:CE1	1:A:163:LYS:HD2	2.55	0.41
1:B:35:ILE:O	1:B:38:ARG:HG2	2.20	0.41
1:A:903:GLN:O	1:A:905:ASP:N	2.52	0.41
1:C:220:THR:O	1:C:224:LEU:HD13	2.20	0.41
1:C:306:SER:HA	1:D:315:LEU:HD21	2.02	0.41
1:A:35:ILE:O	1:A:38:ARG:HG2	2.20	0.41
1:A:268:TYR:CZ	1:D:290:ARG:NH2	2.88	0.41
1:A:216:LEU:CD1	1:A:225:VAL:CG2	2.87	0.41
1:C:35:ILE:O	1:C:38:ARG:HG2	2.20	0.41
1:C:157:PHE:CE1	1:C:163:LYS:HD2	2.56	0.41
1:A:430:ILE:CG2	1:B:844:LEU:HD21	2.51	0.41
1:A:462:PRO:HG2	1:B:903:GLN:CG	2.44	0.41
1:B:157:PHE:CE1	1:B:163:LYS:HD2	2.56	0.41
1:A:901:LEU:N	1:A:901:LEU:HD12	2.36	0.41
1:C:902:ASP:OD1	1:C:903:GLN:N	2.53	0.41
1:D:35:ILE:O	1:D:38:ARG:HG2	2.20	0.41
1:C:216:LEU:HD11	1:C:225:VAL:CG2	2.35	0.40
1:A:220:THR:O	1:A:224:LEU:HD13	2.20	0.40
1:D:157:PHE:CE1	1:D:163:LYS:HD2	2.56	0.40
1:A:315:LEU:HD21	1:D:306:SER:HA	2.02	0.40
1:B:908:ASP:HB2	1:B:911:THR:HG23	2.04	0.40
1:C:738:ARG:CB	1:C:818:LEU:HD13	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	887/1065 (83%)	840 (95%)	46 (5%)	1 (0%)	48 79
1	B	887/1065 (83%)	838 (94%)	47 (5%)	2 (0%)	43 74
1	C	887/1065 (83%)	838 (94%)	49 (6%)	0	100 100
1	D	887/1065 (83%)	838 (94%)	49 (6%)	0	100 100
All	All	3548/4260 (83%)	3354 (94%)	191 (5%)	3 (0%)	49 79

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	710	SER
1	A	904	ASP
1	B	905	ASP

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	765/931 (82%)	760 (99%)	5 (1%)	76 78
1	B	765/931 (82%)	755 (99%)	10 (1%)	61 72
1	C	765/931 (82%)	760 (99%)	5 (1%)	76 78
1	D	765/931 (82%)	760 (99%)	5 (1%)	76 78
All	All	3060/3724 (82%)	3035 (99%)	25 (1%)	70 77

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	201	LEU
1	A	203	LEU
1	A	420	GLN
1	A	580	ILE
1	A	709	ASP
1	B	201	LEU
1	B	203	LEU
1	B	420	GLN
1	B	580	ILE
1	B	709	ASP
1	B	902	ASP
1	B	904	ASP
1	B	905	ASP
1	B	906	ASP
1	B	908	ASP
1	C	201	LEU
1	C	203	LEU
1	C	420	GLN
1	C	580	ILE
1	C	709	ASP
1	D	201	LEU
1	D	203	LEU
1	D	420	GLN
1	D	580	ILE
1	D	709	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	243	HIS
1	A	247	ASN
1	A	386	GLN
1	A	429	ASN
1	A	460	ASN
1	A	739	ASN
1	A	758	ASN
1	A	831	ASN
1	A	1016	HIS
1	B	243	HIS
1	B	247	ASN
1	B	333	HIS
1	B	386	GLN
1	B	429	ASN

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Mol	Chain	Res	Type
1	B	438	ASN
1	B	460	ASN
1	B	739	ASN
1	B	758	ASN
1	B	1016	HIS
1	C	243	HIS
1	C	247	ASN
1	C	333	HIS
1	C	386	GLN
1	C	429	ASN
1	C	453	HIS
1	C	460	ASN
1	C	739	ASN
1	C	758	ASN
1	C	831	ASN
1	C	1016	HIS
1	D	243	HIS
1	D	247	ASN
1	D	333	HIS
1	D	386	GLN
1	D	429	ASN
1	D	453	HIS
1	D	460	ASN
1	D	739	ASN
1	D	758	ASN
1	D	831	ASN
1	D	903	GLN
1	D	1016	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

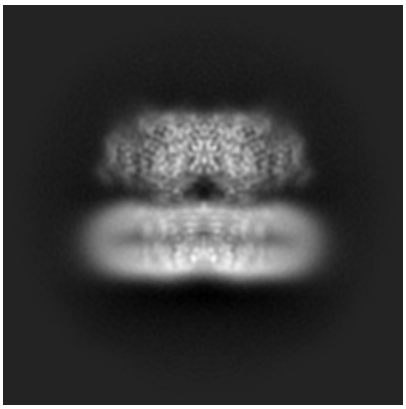
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-46963. These allow visual inspection of the internal detail of the map and identification of artifacts.

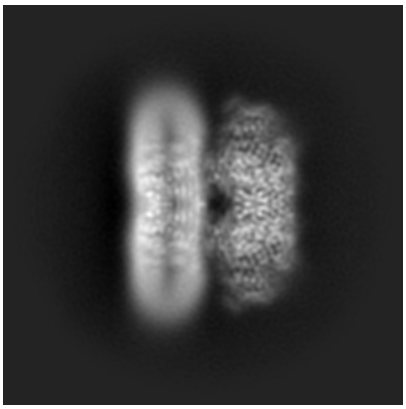
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

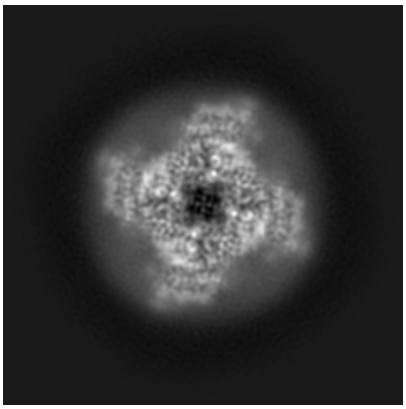
6.1.1 Primary map



X

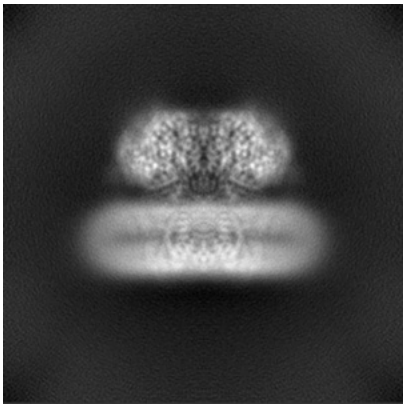


Y

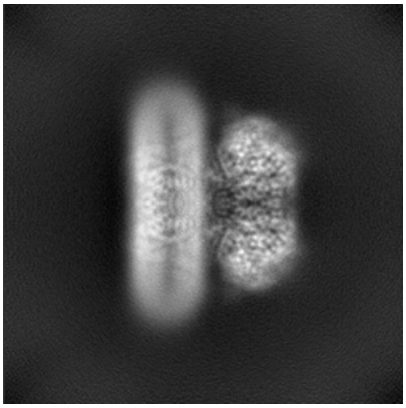


Z

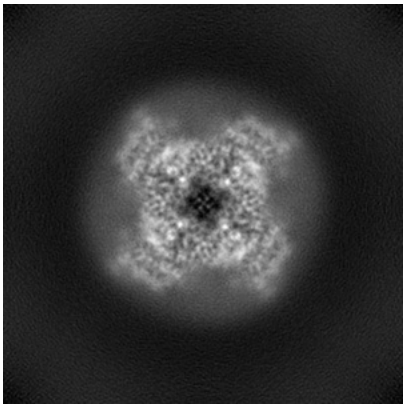
6.1.2 Raw map



X



Y

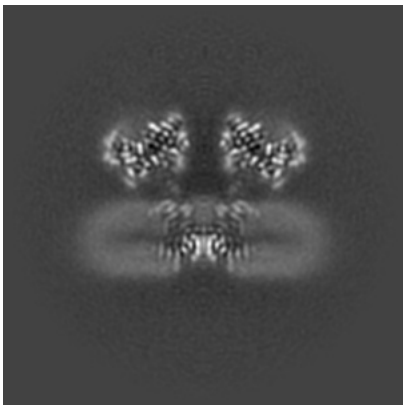


Z

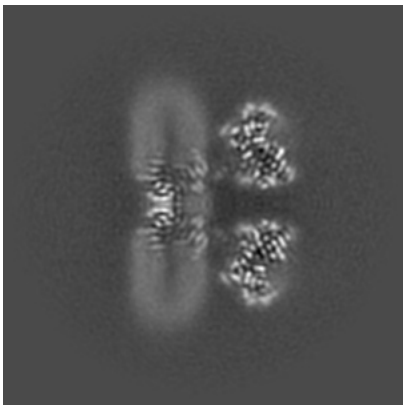
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

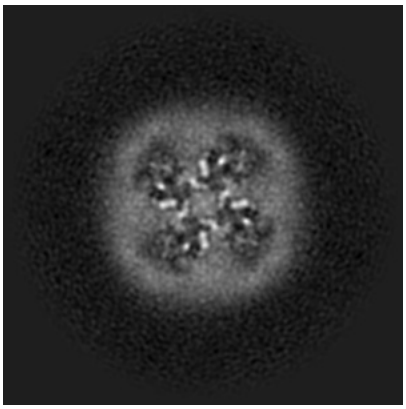
6.2.1 Primary map



X Index: 128

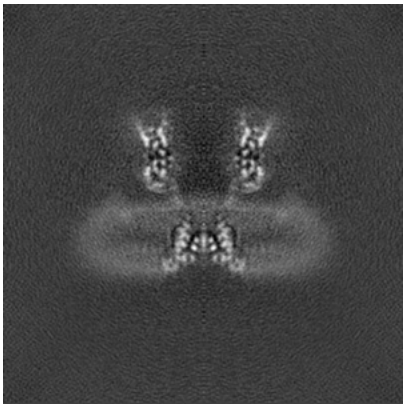


Y Index: 128

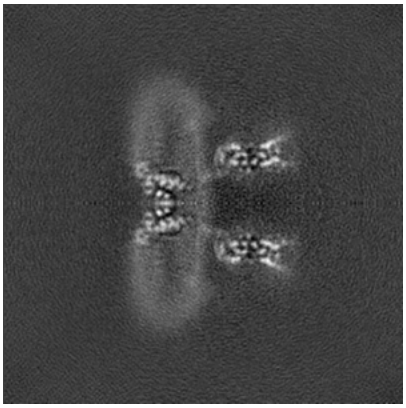


Z Index: 128

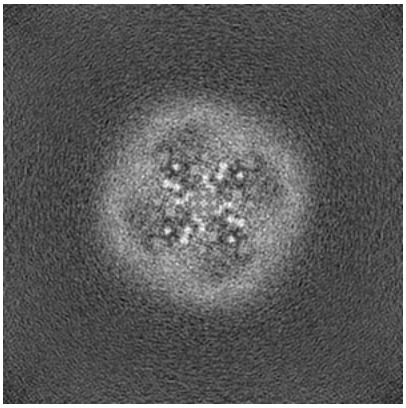
6.2.2 Raw map



X Index: 128



Y Index: 128

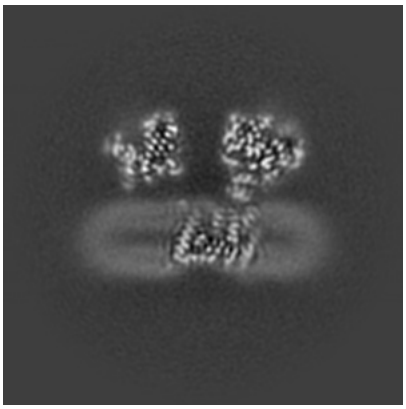


Z Index: 128

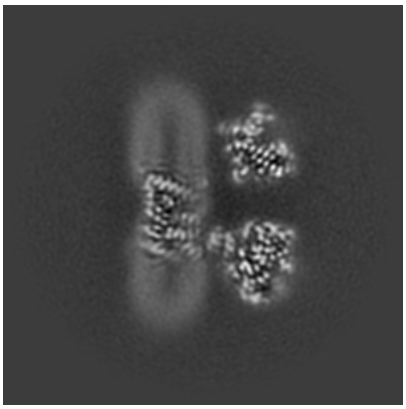
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

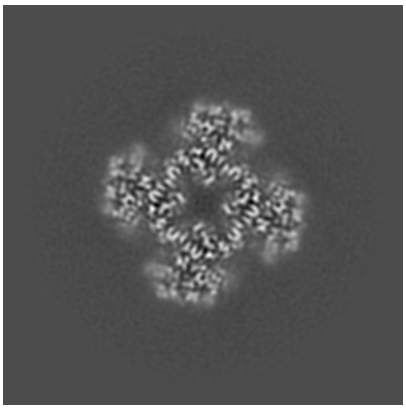
6.3.1 Primary map



X Index: 134

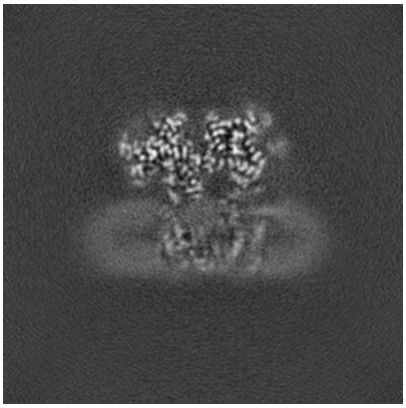


Y Index: 134

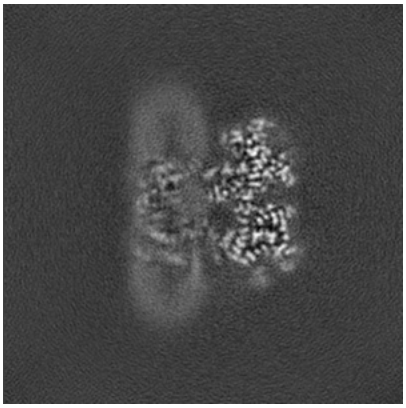


Z Index: 163

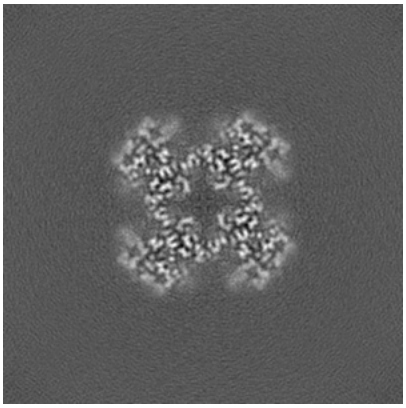
6.3.2 Raw map



X Index: 106



Y Index: 106

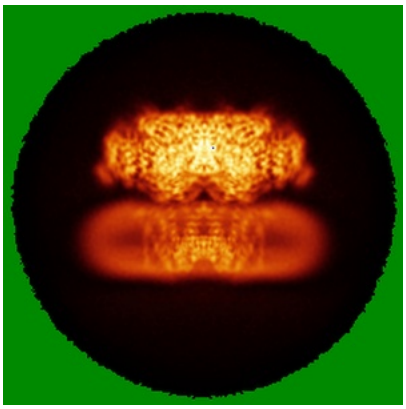


Z Index: 164

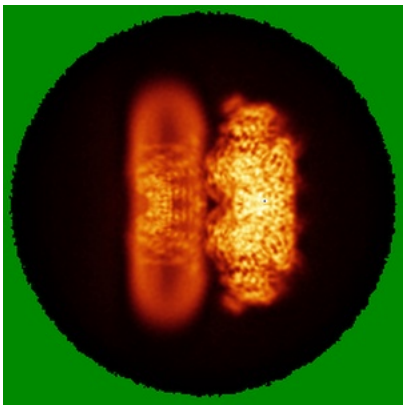
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

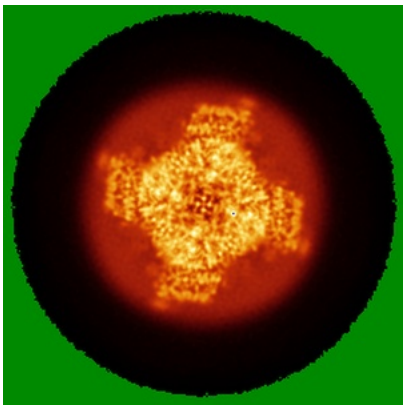
6.4.1 Primary map



X

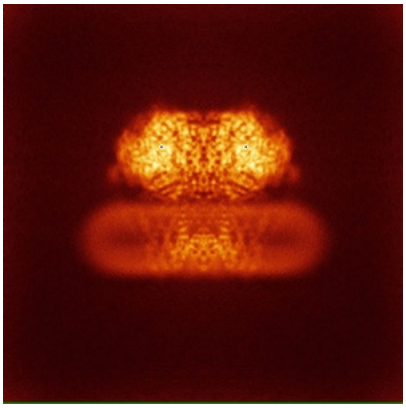


Y

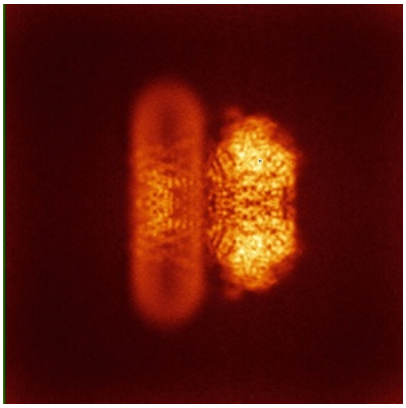


Z

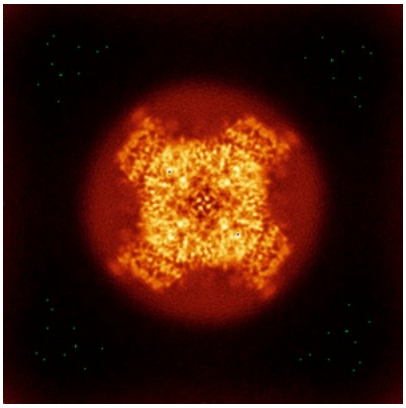
6.4.2 Raw map



X



Y

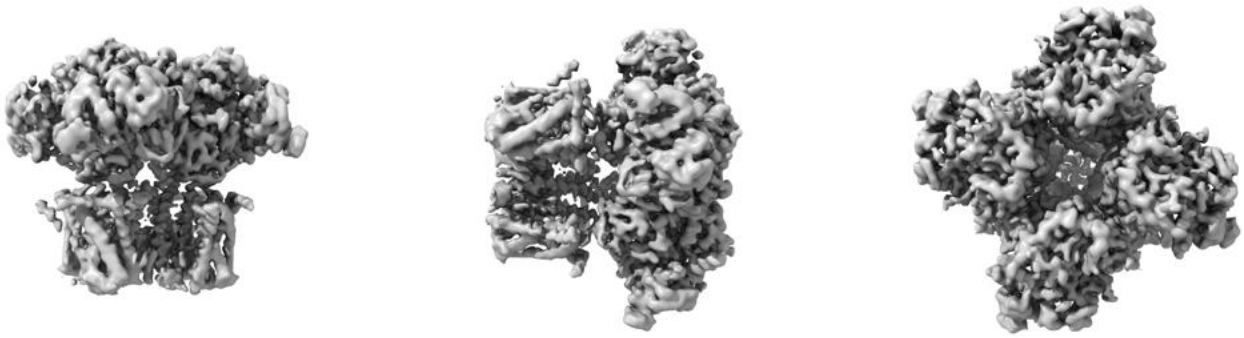


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.259. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

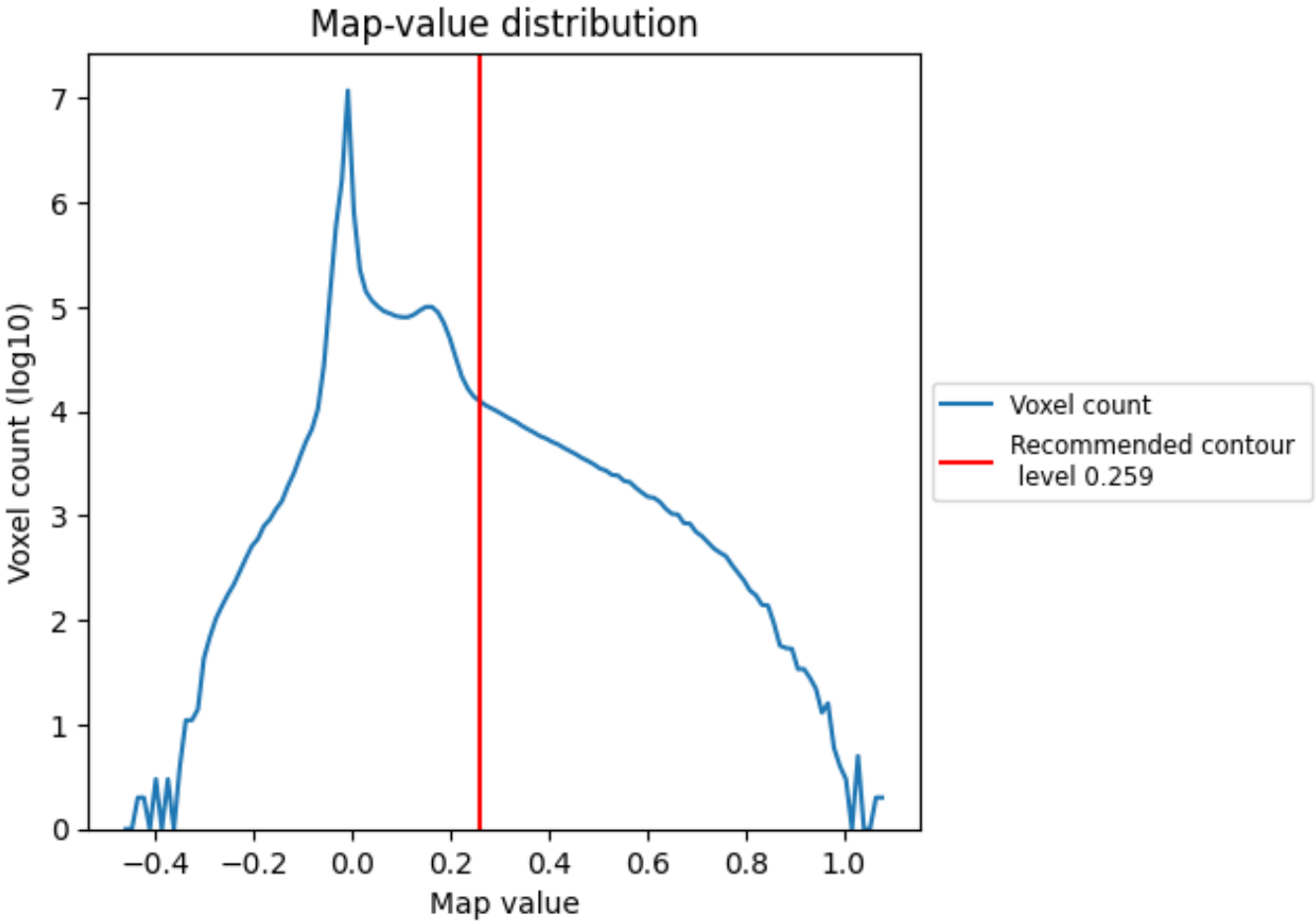
6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

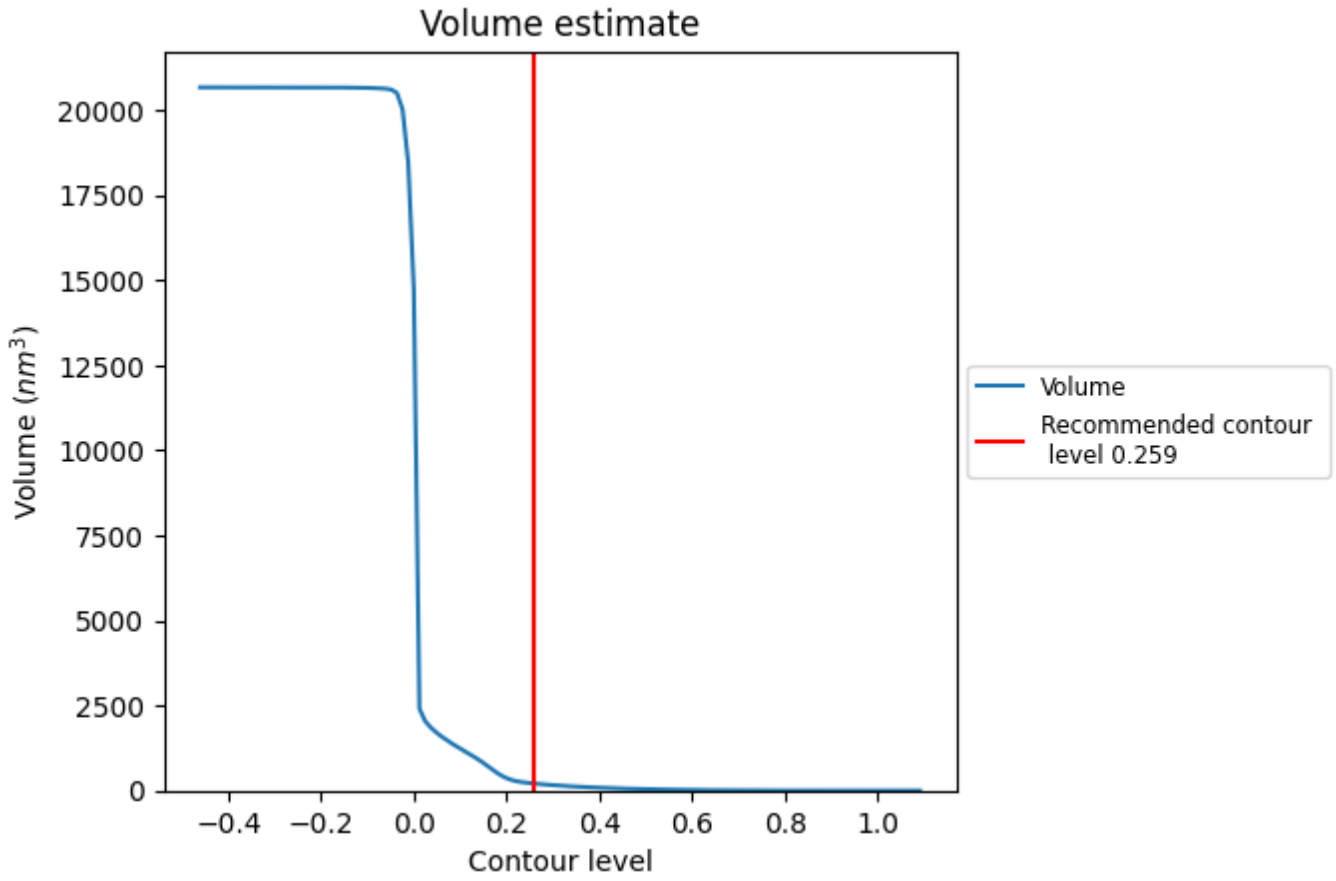
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

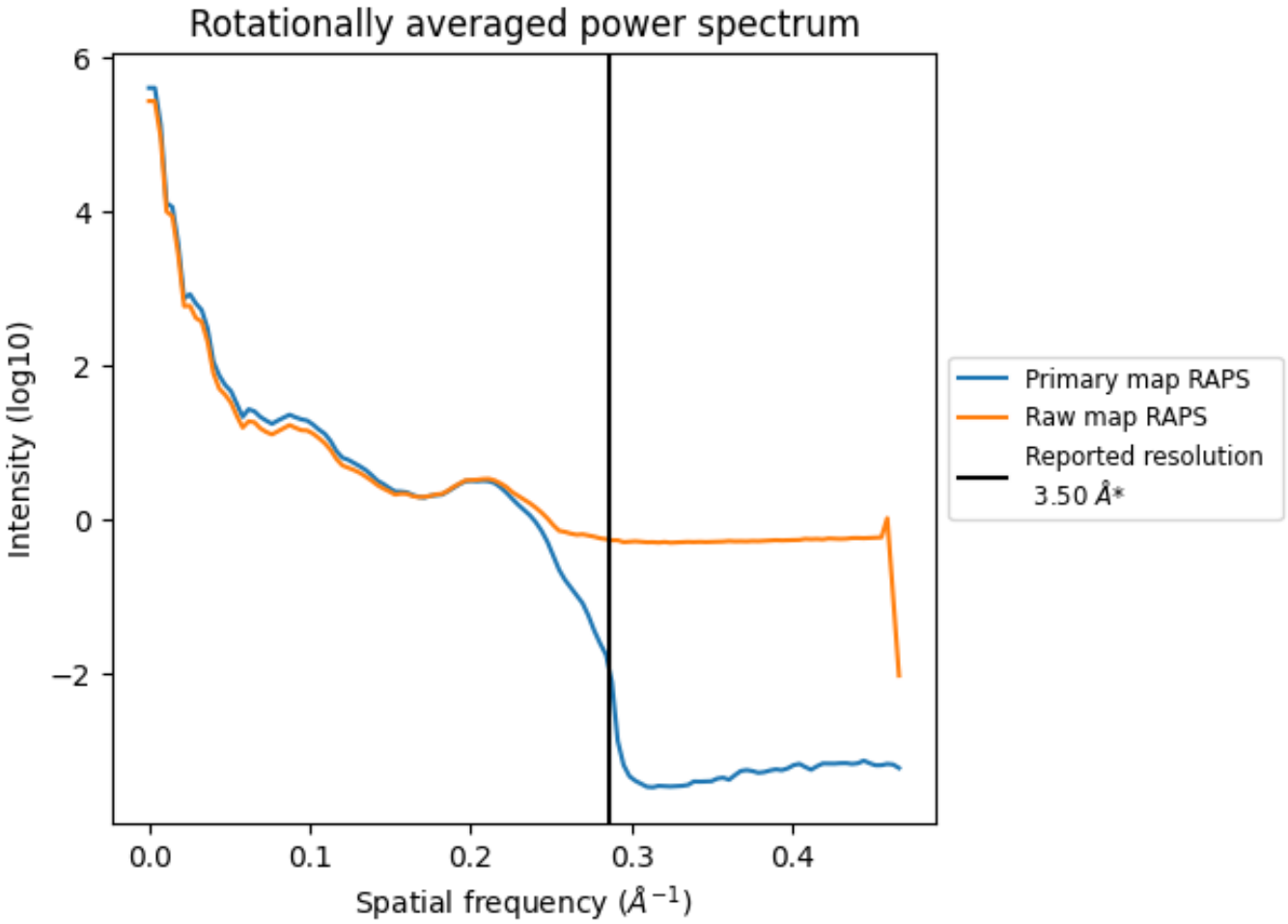
7.2 Volume estimate



The volume at the recommended contour level is 206 nm^3; this corresponds to an approximate mass of 186 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

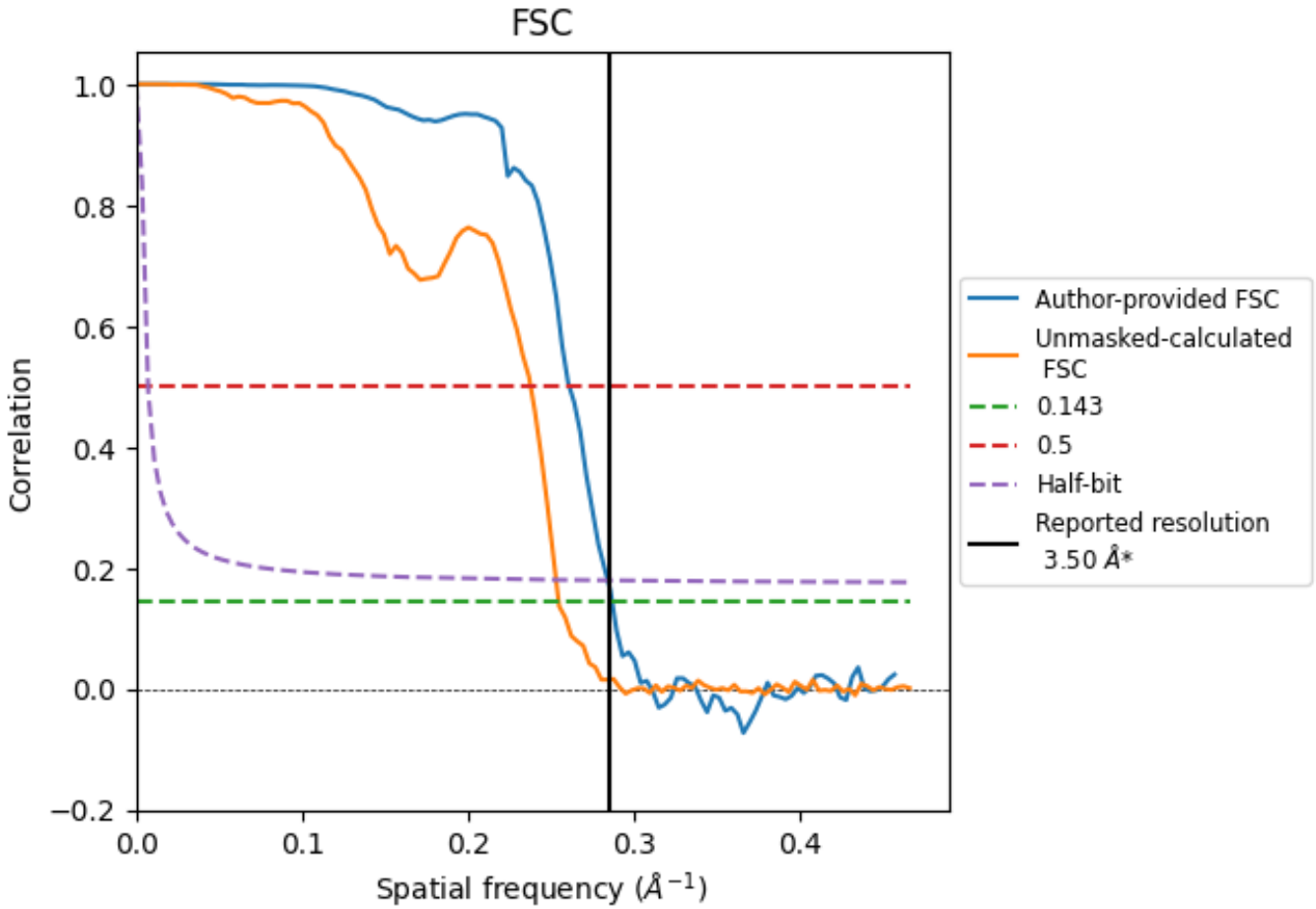


*Reported resolution corresponds to spatial frequency of 0.286 $Å^{-1}$

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

8.2 Resolution estimates (i)

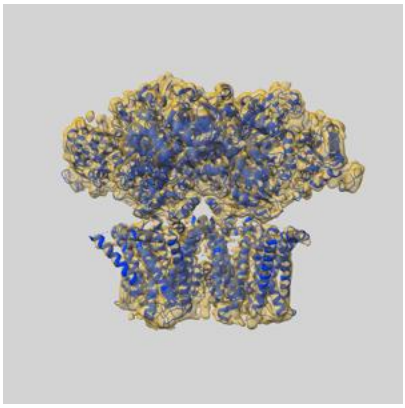
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.48	3.83	3.52
Unmasked-calculated*	3.92	4.20	3.95

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.92 differs from the reported value 3.5 by more than 10 %

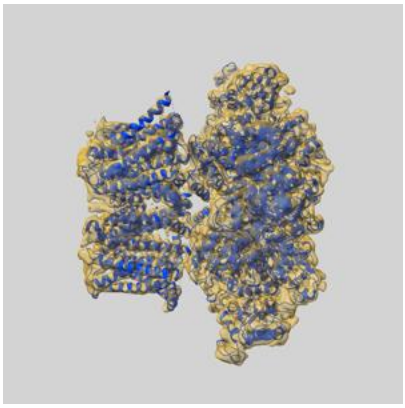
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-46963 and PDB model 9DKN. Per-residue inclusion information can be found in section 3 on page 4.

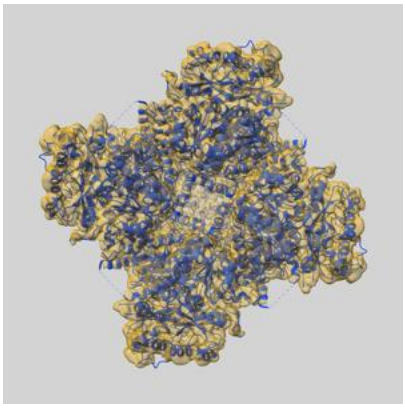
9.1 Map-model overlay



X



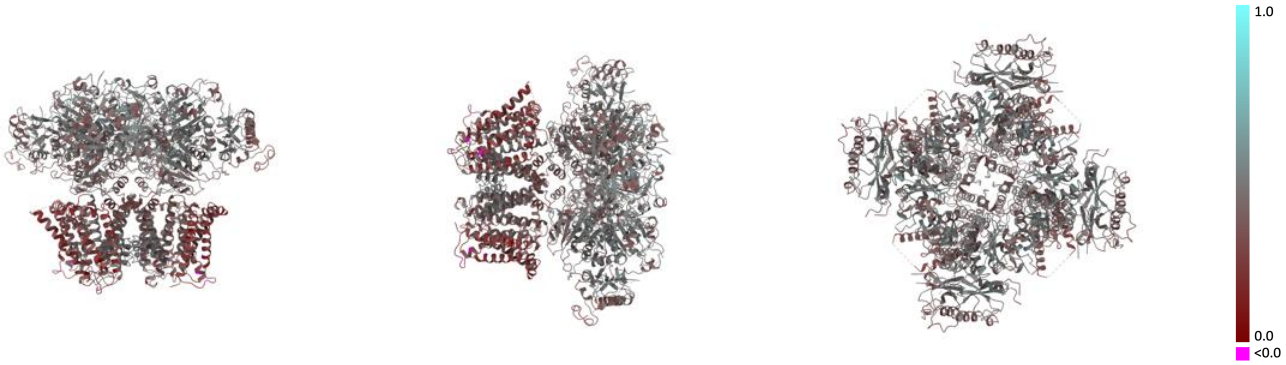
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.259 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

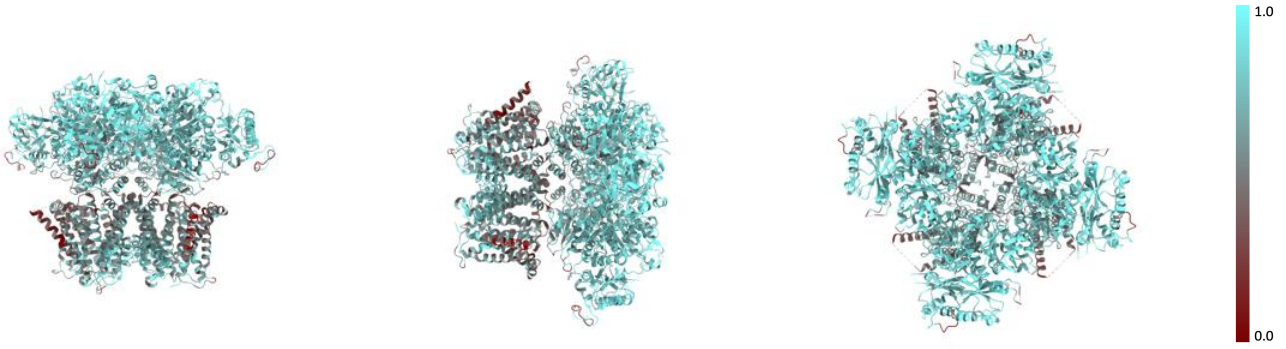
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

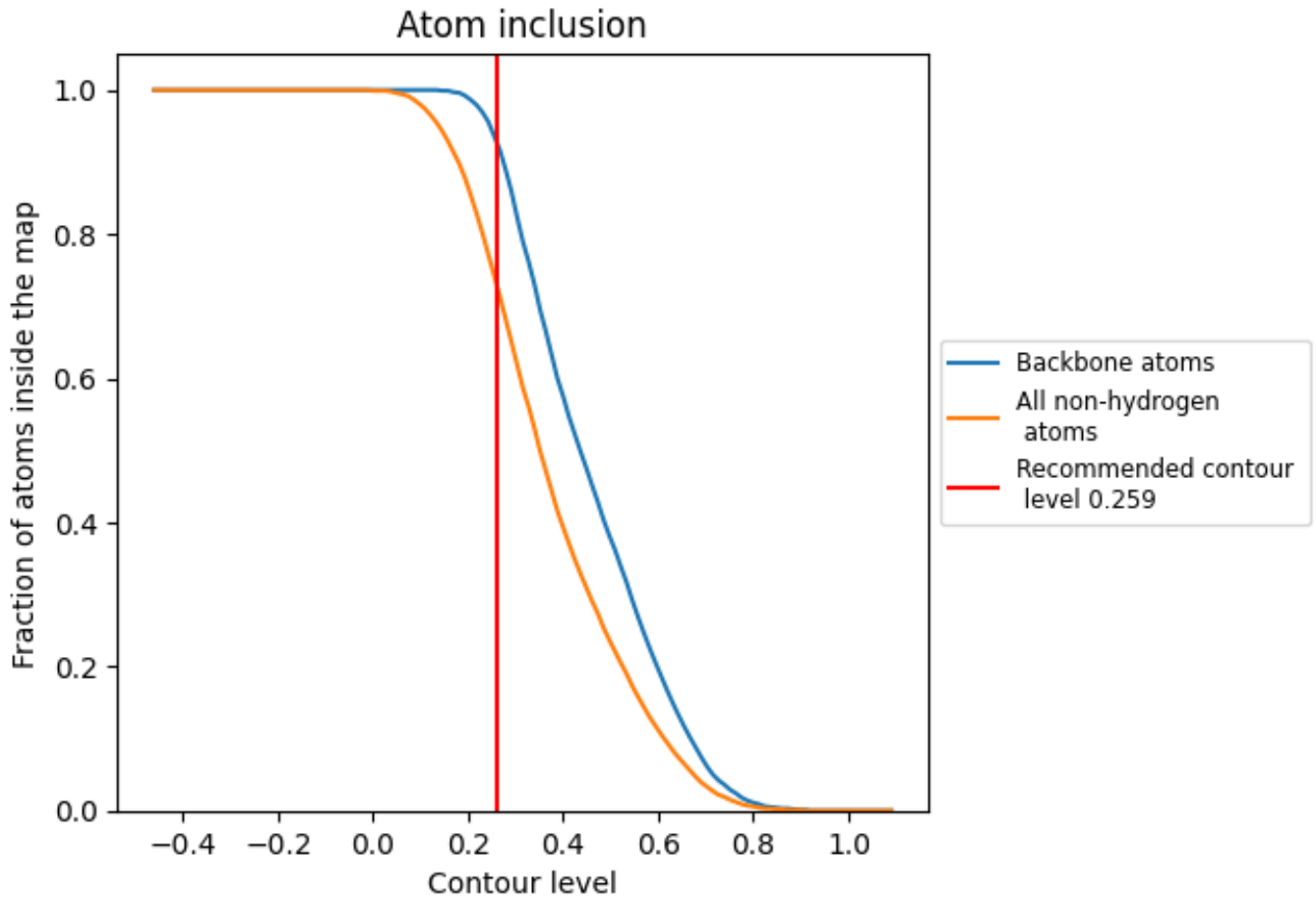
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.259).

9.4 Atom inclusion (i)



At the recommended contour level, 93% of all backbone atoms, 73% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.259) and Q-score for the entire model and for each chain.



Chain	Atom inclusion	Q-score
All	0.7310	0.4020
A	0.7330	0.4040
B	0.7300	0.4010
C	0.7320	0.4030
D	0.7300	0.4000